Matt I J Probert

List of Publications by Year
in descending order

58 papers	21,685 citations	430442 18 h-index	149479 56 g-index
76 all docs	76 docs citations	76 times ranked	19812 citing authors

#	Article	IF	Citations
1	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
2	First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics Condensed Matter, 2002, 14, 2717-2744.	0.7	8,382
3	Exploring atomic defects in molybdenum disulphide monolayers. Nature Communications, 2015, 6, 6293.	5.8	1,124
4	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
5	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
6	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
7	Improving the convergence of defect calculations in supercells: Anab initiostudy of the neutral silicon vacancy. Physical Review B, 2003, 67, .	1.1	163
8	A periodic genetic algorithm with real-space representation for crystal structure and polymorph prediction. Physical Review B, 2006, 73, .	1.1	145
9	Langevin dynamics in constant pressure extended systems. Journal of Chemical Physics, 2004, 120, 11432-11441.	1.2	116
10	Quantum Nature of the Proton in Water-Hydroxyl Overlayers on Metal Surfaces. Physical Review Letters, 2010, 104, 066102.	2.9	101
11	Stiffness and thermal expansion of ZrB2: anab initiostudy. Journal of Physics Condensed Matter, 2005, 17, 2233-2241.	0.7	85
12	Quantum simulation of low-temperature metallic liquid hydrogen. Nature Communications, 2013, 4, 2064.	5.8	75
13	Improved real-space genetic algorithm for crystal structure and polymorph prediction. Physical Review B, 2008, 77, .	1.1	37
14	Huge power factor in p-type half-Heusler alloys NbFeSb and TaFeSb. JPhys Materials, 2019, 2, 035002.	1.8	33
15	Crystal structure prediction for iron as inner core material in heavy terrestrial planets. Earth and Planetary Science Letters, 2011, 312, 237-242.	1.8	32
16	DL_MG: A Parallel Multigrid Poisson and Poissonâ€“Boltzmann Solver for Electronic Structure Calculations in Vacuum and Solution. Journal of Chemical Theory and Computation, 2018, 14, 1412-1432.	2.3	31
17	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. Journal of Physics Condensed Matter, 2013, 25, 085402.	0.7	25
18	The emergence of sequence-dependent structural motifs in stretched, torsionally constrained DNA. Nucleic Acids Research, 2020, 48, 1748-1763.	6.5	21

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19	Many-body renormalization of forces in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> -electron materials. Physical Review B, 2018, 98, .	1.1	20
20	Anab initiostudy of xenon retention in Î±-quartz. Journal of Physics Condensed Matter, 2010, 22, 025501.	0.7	19
21	Anisotropy in antiferromagnets. Journal of Applied Physics, 2020, 128, .	1.1	19
22	Atomistic dynamics of sulfur-deficient high-symmetry grain boundaries in molybdenum disulfide. Nanoscale, 2017, 9, 10312-10320.	2.8	18
23	Phase behavior of a three-dimensional core-softened model system. Physical Review E, 2005, 71, 065701.	0.8	16
24	Improved algorithm for geometry optimisation using damped molecular dynamics. Journal of Computational Physics, 2003, 191, 130-146.	1.9	15
25	Nature of the Irreversibility Line in High-Temperature Superconductors. Physical Review Letters, 1995, 75, 1835-1838.	2.9	14
26	Experimental and density functional study of Mn doped Bi2Te3 topological insulator. APL Materials, 2016, 4, .	2.2	14
27	Constant pressure Langevin dynamics: theory and application. Computer Physics Communications, 2005, 169, 322-325.	3.0	13
28	The structure and growth direction of rare earth silicide nanowires on Si(100). Applied Physics Letters, 2010, 96, 241903.	1.5	13
29	Off-the-shelf DFT-DISPersion methods: Are they now â€œon-trendâ€•for organic molecular crystals?. Journal of Chemical Physics, 2019, 151, 044106.	1.2	11
30	Atomistic molecular dynamics simulations of shock compressed quartz. Journal of Chemical Physics, 2011, 135, 044508.	1.2	9
31	The Effect of Cobalt-Sublattice Disorder on Spin Polarisation in Co2FexMn1â^'xSi Heusler Alloys. Materials, 2014, 7, 1473-1482.	1.3	9
32	Quantitative LEEDIâ^'Vandab initiostudy of theSi(111)â^'3Ã—2â^'Smsurface structure and the missing half-order spots in the3Ã—1diffraction pattern. Physical Review B, 2007, 75, .	1.1	8
33	Simultaneous Prediction of the Magnetic and Crystal Structure of Materials Using a Genetic Algorithm. Crystals, 2019, 9, 439.	1.0	8
34	Potential for a novel Î¼SR experiment â€" the results of an ab initio study. Chemical Physics Letters, 1996, 259, 271-275.	1.2	7
35	Materials and Molecular Modeling at the Exascale. Computing in Science and Engineering, 2022, 24, 36-45.	1.2	7
36	Anab initiostudy of muons in ethanal. Journal of Physics Condensed Matter, 1997, 9, 3241-3257.	0.7	6

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37	STM andab initiostudy of holmium nanowires on a Ge(111) surface. Physical Review B, 2006, 74, .	1.1	6
38	Non-equilibrium electron transport in degenerate nitride heterostructuresâ€"dynamic screening effects. Physica E: Low-Dimensional Systems and Nanostructures, 2003, 17, 272-275.	1.3	5
39	Theoretical study of core-loss electron energy-loss spectroscopy at graphene nanoribbon edges. Journal of Physics Condensed Matter, 2015, 27, 305301.	0.7	5
40	Electronâ€"phonon interaction and superconductivity in hexagonal ternary carbides Nb₂ AC (A: Al, S, Ge, As and Sn). Electronic Structure, 2021, 3, 045001.	1.0	5
41	Systematic Comparison of Genetic Algorithm and Basin Hopping Approaches to the Global Optimization of Si(111) Surface Reconstructions. Journal of Physical Chemistry A, 2022, 126, 3043-3056.	1.1	5
42	Ab initiostudies of magnetism in the organic radicalp-NPNN. Journal of Physics Condensed Matter, 1997, 9, 3635-3645.	0.7	4
43	Progression of phase behavior for a sequence of model core-softened potentials. Physical Review E, 2005, 72, 061202.	0.8	4
44	Quantum diffusion of H/D on Ni(111)â€"A partially adiabatic centroid MD study. Journal of Chemical Physics, 2018, 148, 102339.	1.2	4
45	Effective modelling of the Seebeck coefficient of Fe₂VAl. Journal of Physics Condensed Matter, 2020, 32, 125401.	0.7	4
46	Theoretical studies of implanted muons in organic magnets. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 247-250.	1.7	3
47	Comment on â€œAlgorithm for normal random numbersâ€• Physical Review E, 2001, 63, 058701; author reply 058702.	0.8	3
48	An experiment on the Purcell effect in a wedge cavity. European Journal of Physics, 2009, 30, S81-S88.	0.3	3
49	Orientational effects of twisted light on twisted nematic liquid crystals. Journal of Physics B: Atomic, Molecular and Optical Physics, 2006, 39, S523-S528.	0.6	2
50	Comment on `Checking the influence of numerically induced chaos in the computational study of intramolecular dynamics using trajectory equivalence'. Chemical Physics Letters, 2002, 354, 529-531.	1.2	1
51	Molecular dynamics studies of liquids using a Beowulf computer. Contemporary Physics, 2003, 44, 435-450.	0.8	1
52	Computer simulations of flux motion in high-temperature superconductors. Physica B: Condensed Matter, 1995, 205, 180-182.	1.3	0
53	Ab Initio Path Integral Molecular Dynamics Simulation of Hydrogen in Silicon. AIP Conference Proceedings, 2006, , .	0.3	0
54	Hydrogen sorption sites in holmium silicide on silicon(1 1 1). Surface Science, 2010, 604, 686-691.	0.8	0

#	Article	IF	Citations
55	3rd Workshop on Theory, Modelling and Computational Methods for Semiconductors (TMCSIII). Journal of Physics: Conference Series, 2012, 367, 011001.	0.3	0
56	4th Workshop on Theory, Modelling and Computational Methods for Semiconductors (TMCSIV). Journal of Physics: Conference Series, 2014, 526, 011001.	0.3	0
57	Transverse Fluorescence Microscopy with Magnetic and Optical Tweezers. Biophysical Journal, 2017, 112, 299a.	0.2	0
58	Theory, Modelling and Computational methods for Semiconductors. Journal of Physics: Conference Series, 2010, 242, 011001.	0.3	0